

Conservative Semi-Lagrangian Reconstructions

Oleg Kravchenko¹ & Manuel Diaz*

¹ Department of Higher Mathematics, Bauman Moscow State Technical University, Moscow, Russia.

* Institute of Applied Mechanics, National Taiwan University, Taiwan R.O.C.

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Abstract

A class of high-order constrained reconstructions, in the context of finite difference methods for scalar hyperbolic conservation laws, are presented and numerically studied in the presence of local extrema, or shock solutions. Although these reconstructions can use large time steps given their semi-Lagrangian in nature, a conservative formulation of the conservation is here considered. The numerical one-dimensional implementations in Matlab are reported to provide a simple follow up of the formulations here versed. Application to the nonlinear Boltzmann-BGK equation to model the dynamics of inert gas flows in near continuum regimes are explored.

1 Introduction

The semi-Lagrangian method is a numerical solution technique for the partial differential equations describing the advection process. It accounts for the Lagrangian nature of the transport process but, at the same time, it allows to work on a fixed computational grid. Starting from the first proposals to in the meteorological literature, which focused on the advection of vorticity in simplified models of large scale flow, it has developed into a mature discretization approach for the complete equations of atmospheric flows. The semi-Lagrangian is also related (and, in some cases, entirely equivalent) to similar methods developed in other modelling communities, such as for example the modified method of characteristics, the Eulerian-Lagrangian method, the characteristic Galerkin method and the constrained interpolation polynomial methods. This last, have been proved to achieve excellent results for scalar conservation laws.

Much work has been done in the text of semi-lagrangian constrained reconstructions with polynomials, here we point some of our observations:

- Yabe and Aoki (1991) introduced the initial concept of cubic interpolation polynomial (CIP) for the evolution of scalar advection equations considering the also the evolution of the cell averages slope information. This simple idea has been proved to be workable but conservation cannot be guaranteed.
- Two years later Yabe et al. (2001), introduced a new reformulation of their CIP algorithm which now considers the cell numerical-mass conservation as a constrain and a reconstruction of a flux as and integral function is introduced in this semi-Lagrangian formulation.

- Conservative formulation of CIP methods where first introduced by Tanaka et al. (2000) and Xiao and Yabe (2001).
- Extension to multi-dimensional formulation of the CIP algorithms where reported by Nakamura et al. (2001).

It is interesting to point out the conceptual similarities of CIP-CSL schemes in Ii and Xiao (2007) with the *flux reconstruction* (FR) schemes by Huynh (2007). As both formulation achieve successfully high-order and accurate representations. However a clear advantage of the CIP-CSL is the simple incorporation of slope limiters in to the formulation which in the context of FR schemes breaks the abstraction of correction functions. Moreover, although their success the numerical experience of these methods reveals that both implementations require fast computational resources as their stability conditions can only allow small time steps. The above is also result of the fact that CIP-CSL and FR are closer to an Eulerian description of flow conditions, see for example Ii and Xiao (2009).

It is found that CIP literature is rich in ideas and strategies to ensure the conservative properties of the method, improve their accuracy or deal with the oscillations that arise near local extrema. We notice that CIP implementation with rational functions by Xiao et al. (1996). Here the use of such function instead of polynomials led to limiter free CIP second-order implementation that can deal with discontinuities in the solution in a straight manner. This observation resonates with the *local dual logarithmic reconstructions* (LDLR) by Artebrant and Schroll (2006). Which led us to consider a non-polynomial reconstructions to formulate new semi-Lagrangian reconstruction that can handle discontinuities that arise with the solutions in a much straight and computationally economic manner.

The present document is , section 4 introduces the basic formulation of CIP by Yabe and Aoki (1991), followed by its modification to a fully conservative semi-Lagrangian scheme in section 5. In section 6 the concept of constrained interpolation is considered with a non-polynomial function. Lastly, some concluding remarks are given section 7.

2 Accuracy of Polynomial and non-Polynomial Interpolation Functions

Lemma 1. Consider a given function f and denote g as an approximation of f such that $g \in C^3[a, b]$, with $\Delta = b - a$. Assuming that an integral relation of the form

$$\int_a^b f(x)dx = \int_a^b g(x)dx, \quad (1)$$

hold and that the lateral gradient agree up to second-order

$$(f - g)'(a) = \mathcal{O}(\Delta x^2) = (f - g)'(b), \quad (2)$$

then, $(f - g)(x) = \mathcal{O}(\Delta x^3)$ for all $x \in [a, b]$.

Proof. We define $w(x) \equiv (f - g)(x)$. A Taylor expansion around $x' \in [a, b]$ yields

$$w(x) = w(x') + w'(x')(x - x') + \frac{1}{2}w''(x')(x - x')^2 + \mathcal{O}(|x - x'|^3), \quad (3)$$

for an arbitrary $x \in [a, b]$. By continuity of f , g and because of $\int_a^b w(x)dx = 0$, we know that there exist a $x' \in [a, b]$, such that

$$w(x') = 0. \quad (4)$$

The mean value theorem implies that

$$w''(x') = \frac{w'(a) - w'(b)}{\Delta x}, \quad (5)$$

for $x' \in [a, b]$ and $\Delta x = b - a$. With assumption (2) it follows that $w''(x') = \mathcal{O}(\Delta x)$. A Taylor expansion of $w'(x')$ around a yields

$$w'(x') = x'(a) + \mathcal{O}(|x' - a|^2) = \mathcal{O}(\Delta x^2), \quad (6)$$

since $w'(a) = \mathcal{O}(\Delta x^2)$ and $w''(a) = \mathcal{O}(\Delta x)$. Consequently we get

$$w(x) \equiv (f - g)(x) = \mathcal{O}(\Delta x^3), \quad (7)$$

which concludes the proof. \square

Note that g function must not be necessarily a polynomial. In fact one can use any function $g_i(x)$, for which holds $g_i(x) \in C^3[x_{i-1/2}, x_{i+1/2}]$ for all i -cells.

3 3rd Order Interpolation Polynomials

Three data points are sufficient for constructing a unique quadratic interpolation function with the Ansatz function

$$p_i(x) = a_i + b_i(x - x_i) + \frac{c_i}{2}(x - x_i)^2. \quad (8)$$

To derive the coefficients a_i , b_i and c_i we impose the conditions set in Lemma 1. Therefore the quadratic function $p_i(x)$, integrated over the cell $C_i = [x_{i-1/2}, x_{i+1/2}]$ has to recover the cell average \bar{u} itself and its left and right derivatives located at the cell interfaces have to be approximated to second order $\mathcal{O}(\Delta x^2)$.

Given the set of cell averages $\bar{u}_{i-1}, \bar{u}_i, \bar{u}_{i+1}$ we require

$$\frac{1}{\Delta x} \int_{C_i} p_i(x) dx = \bar{u}_i, \quad (9)$$

$$p'_i(x_i - \Delta x/2) = d_1 = \frac{\bar{u}_{i+1} - \bar{u}_i}{\Delta x}, \quad (10)$$

$$p'_i(x_i + \Delta x/2) = d_2 = \frac{\bar{u}_i - \bar{u}_{i-1}}{\Delta x}. \quad (11)$$

The above

$$a_i = \bar{u}_i - \frac{1}{24}(\bar{u}_{i+1} - \bar{u}_i + \bar{u}_{i-1}), \quad (12)$$

$$b_i = \frac{1}{2\Delta x}(\bar{u}_{i+1} - \bar{u}_{i-1}), \quad (13)$$

$$c_i = \frac{1}{\Delta x^2}(\bar{u}_{i+1} - \bar{u}_i + \bar{u}_{i-1}). \quad (14)$$

Evaluating the polynomial (8) at the cell boundaries yields

$$\hat{u}_{i+\frac{1}{2}}^{(-)} \equiv p_i(x_{i+1/2}) = -\frac{1}{6}\bar{u}_{i-1} + \frac{5}{6}\bar{u}_i + \frac{1}{3}\bar{u}_{i+1}, \quad (15)$$

$$\hat{u}_{i-\frac{1}{2}}^{(+)} \equiv p_i(x_{i-1/2}) = \frac{1}{3}\bar{u}_{i-1} + \frac{5}{6}\bar{u}_i - \frac{1}{6}\bar{u}_{i+1}. \quad (16)$$

The idea of high-order polynomial reconstruction goes back to Van Leer (1974). Van Leer published in a series of papers different local reconstructions functions including the quadratic interpolation. The schemes developed by Van Leer are second order accurate on smooth regions of the solution, yet does not produce any spurious oscillations at jump discontinuities. Such methods, are now known as *shock capturing schemes*.

4 Constrained Interpolation Polynomials

Consider a scalar conservation law of the form

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = 0, \quad \text{for } x \in \Omega \in \mathbb{R}, t \geq 0, \quad (17)$$

where $f : f(x, t)$ indicates a scalar field define in the domain Ω and to be transported in time. $v(x, t) \in \mathbb{R}$ is the characteristic advection speed. Let us now consider denote $g = \frac{\partial f}{\partial x}$ as the slope of the scalar field f .

Taking the derivative of equation (17) with respect to x yields

$$\frac{\partial}{\partial x} \left(\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} \right) = \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial t} \right) + \frac{\partial v}{\partial x} \left(\frac{\partial f}{\partial x} \right) + v \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial x} \right) = 0, \quad (18)$$

under the assumption of a constant velocity field v , the above result simply reduces to

$$\frac{\partial g}{\partial t} + v \frac{\partial g}{\partial x} = 0 \quad (19)$$

if both values of f and g are given at the cell boundaries, the profile of every cell can be reconstructed by an interpolation using a cubic polynomial

$$F(x) = a \left(x - x_{i-\frac{1}{2}} \right)^3 + b \left(x - x_{i-\frac{1}{2}} \right)^2 + c \left(x - x_{i-\frac{1}{2}} \right) + d \quad (20)$$

where a , b , c and d are to be defined under the constrains

$$F(x_{i-\frac{1}{2}}) = f_{i-\frac{1}{2}}, \quad (21)$$

$$F(x_{i+\frac{1}{2}}) = f_{i+\frac{1}{2}}, \quad (22)$$

$$\frac{\partial F}{\partial x} \Big|_{x_{i-\frac{1}{2}}} = g_{i-\frac{1}{2}}, \quad (23)$$

$$\frac{\partial F}{\partial x} \Big|_{x_{i+\frac{1}{2}}} = g_{i+\frac{1}{2}}, \quad (24)$$

$$F(x_i) = f(x_i) = f_i, \quad (25)$$

$$\frac{\partial F}{\partial x} \Big|_{x_i} = g(x_i) = g_i, \quad (26)$$

however notice that under the following constrains the present scheme cannot guarantee conservation of cell average quantities f_i .

5 Conservative semi-Lagrangian Constrained Interpolation Polynomials

Consider a scalar conservation law of the form

$$\frac{\partial f}{\partial t} + \frac{\partial(vf)}{\partial x} = 0, \quad \text{for } x \in \Omega \in \mathbb{R}, t \geq 0, \quad (27)$$

where $f : f(x, t)$ indicates a scalar field define in the domain Ω and to be transported in time. $v(x, t) \in \mathbb{R}$ is the characteristic advection speed. Let us now consider denote $h = \int f dx$ and integrated scalar field of f .

Integrating equation (17) with respect to x yields

$$\int \left(\frac{\partial f}{\partial t} + \frac{\partial(vf)}{\partial x} \right) dx = \frac{\partial}{\partial t} \int f dx + \int \frac{\partial(vf)}{\partial x} dx = 0 \quad (28)$$

under the assumption of a constant velocity field v , the above result simply reduces to

$$\frac{\partial h}{\partial t} + v \frac{\partial h}{\partial x} = 0 \quad (29)$$

since both equations (17) and (29) are the same, the CIP procedure is applied to the pair $\int f dx$ and f instead of f and $\frac{\partial f}{\partial x}$. Using this analogy, h is defined as continuous function defined in the physical space of every cell as

$$h(x) = \int_{x_{i-\frac{1}{2}}}^x f(\xi) d\xi, \quad (30)$$

The profile of every cell can be reconstructed by an interpolation using a cubic polynomial of the form

$$h(x) = a \left(x - x_{i-\frac{1}{2}} \right)^3 + b \left(x - x_{i-\frac{1}{2}} \right)^2 + c \left(x - x_{i-\frac{1}{2}} \right) \quad (31)$$

where a , b and c are to be defined under the constrains

$$h(x_{i-\frac{1}{2}}) = 0, \quad (32)$$

$$h(x_{i+\frac{1}{2}}) = \bar{f}_i \Delta x, \quad (33)$$

$$\frac{\partial h}{\partial x} \Big|_{x_{i-\frac{1}{2}}} = f_{i-\frac{1}{2}}, \quad (34)$$

$$\frac{\partial h}{\partial x} \Big|_{x_{i+\frac{1}{2}}} = f_{i+\frac{1}{2}}, \quad (35)$$

$$\frac{\partial h}{\partial x} \Big|_{x_i} = f(x_i) = f_i, \quad (36)$$

notice that \bar{f}_i denotes the cell average and should not be confused with point value f_i . The cell average is here defined as,

$$\frac{1}{\Delta x_i} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f^n dx = \bar{f}_i^n. \quad (37)$$

6 Conservative semi-Lagrangian Constrained Interpolation non-Polynomials

6.1 Rational Functions

... (comming soon)

6.2 Local Double Logarithmic Reconstruction

The reconstruction functions is this cell has the form

$$r_0(x) \approx A + B \log(x + C) + D \log(x + E), \quad (38)$$

where $x \in C_0$ so that

$$\phi_0(x) = -\frac{c}{a}h \log \left[x - x_0 - \frac{h}{2} \left(\frac{2}{a} - 1 \right) \right] - \frac{d}{b}h \log \left[x - x_0 - \frac{h}{2} \left(\frac{2}{b} - 1 \right) \right], \quad (39)$$

where a, b, c and d are parameters to be determined, and let

$$r_0 = v_0 + \phi_0(x) - \frac{1}{h} \int_{C_0} \phi_0(\xi) d\xi, \quad (40)$$

be the reconstructing function. The reach third order we impose the conditions set in Lema 1, given v_0 , the cell average of the unknown function in C_0 and d_1 and d_2 second order approximations to the left and right derivatives, we require

$$\frac{1}{h} \int_{C_0} r_0(x) dx = v_0, \quad (41)$$

$$\frac{\partial r_0}{\partial x} \left(x_0 - \frac{h}{2} \right) = d_1, \quad (42)$$

$$\frac{\partial r_0}{\partial x} \left(x_0 + \frac{h}{2} \right) = d_2. \quad (43)$$

The reconstruction function (40) preserves the cell averages v_0 by construction. The above conditions lead to the following pair of equations

$$c + d = d_1, \quad (44)$$

$$\frac{d(a-1) + c(b-1)}{(a-1)(b-a)} = d_2. \quad (45)$$

Thus the following four parameters to satisfy two equations. We solve for two parameters, leaving the others undetermined for later use. Solving for c and d yields,

$$c = \frac{(a-1)(d_2(1-b) - d_1)}{b-a}, \quad (46)$$

$$d = d_1 - c. \quad (47)$$

The reconstruction should be symmetric (to the extent allowed by the ansatz function) in the sense that if $r'_0(x_0 - h/2) = -r'_0(x_0 + h/2)$, then $r'(x_0) = 0$. This can be realized by setting $d_1 = -d_2$ and solving for b . We get

$$\frac{\partial r_0(x_0)}{\partial x} \Big|_{d_1=-d_2} = 2d_2 \frac{ab - a - b}{(a-2)(a-1)} = 0, \quad (48)$$

that is,

$$b = \frac{a}{a-1}. \quad (49)$$

Notice that a and b are variables such that $a < 1$ and $b < 1$ and their range goes as $a, b \in (-\infty, 1)$. Also notice that $a = b$ only occurs when $a = b = 0$.

Using the Marquina's concept of local variation boundness (Artebrant and Schroll, 2006), variable a is then defined as

$$a = (1 - tol) \left(1 + tol - \frac{2|d_1|^q |d_2|^q + tol}{|d_1|^{2q} + |d_2|^{2q} + tol} \right). \quad (50)$$

where d_1 and d_2 are first order slopes approximations at the cell boundary. Here, $tol = 0.1h^q$ is a tolerance parameter defined in terms of constant $q = 1.4$ and the cell size $h = (x_{i+1/2} - x_{i-1/2})$.

Using directly the reconstruction function we then obtain

$$r_0(x_0 \pm h/2) = v_0 ch \eta^\pm(a) + dh \eta^\pm(b), \quad (51)$$

where

$$\eta^+(t) = -\frac{\log(1-t) + t}{t^2}, \quad (52)$$

and

$$\eta^+(t) = \frac{(t-1)\log(1-t) - t}{t^2}. \quad (53)$$

Notice in the above that we can exploit the fact

$$\eta^\pm\left(b = \frac{a}{a-1}\right) = (a-1)\eta^\pm(a). \quad (54)$$

The functions η^\pm have a removable singularity at zero by putting $\eta^\pm = \pm\frac{1}{2}$.

7 Concluding Remarks

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